Lecture XVII 49

Lecture XVII: Weakly Interacting Electron Gas: Plasma Theory

▶ How are the properties of an electron gas influenced by weak Coulomb interaction?

▷ QUALITATIVE CONSIDERATIONS:

When is the intereaction weak? Defining $r_0 = \frac{1}{n^{1/3}}$ as the average electron separation, the typical p.e. $\frac{e^2}{r_0}$ and k.e. $\frac{\hbar^2}{mr_0}$ lead to the dimensionless ratio, $r_s = \frac{e^2}{r_0} \frac{mr_0^2}{\hbar^2} \equiv \frac{r_0}{a_0}$, where a_0 is electron Bohr radius, from which one can infer that Coulomb effects dominate at low density

At $r_s \sim 35$ there is (believed to be) a transition to an electron solid phase known as a Wigner crystal (cf. Mott-Hubbard insulator)

For most metals $(2 < r_s < 6)$, k.e. and p.e. comparable; fortunately (thanks to adiabatic continuity) "weak coupling" theory valid even for intermediate r_s

 \triangleright Motivates consideration of weak coupling theory $r_s \ll 1$: Σ -convention on spin

$$\hat{H} = \int d^d r \, c_{\sigma}^{\dagger}(\mathbf{r}) \frac{\hat{\mathbf{p}}^2}{2m} c_{\sigma}(\mathbf{r}) + \frac{1}{2} \int d^d r \int d^d r' c_{\sigma}^{\dagger}(\mathbf{r}) c_{\sigma'}^{\dagger}(\mathbf{r}') \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} c_{\sigma'}(\mathbf{r}') c_{\sigma}(\mathbf{r})$$

Aim: to explore dielectric properties and ground state energy of electron gas through...

▶ QUANTUM PARTITION FUNCTION: using CSPI formulation

$$\mathcal{Z} \equiv \operatorname{tr} \, e^{-\beta(\hat{H}-\mu\hat{N})} = \int_{\substack{\bar{\psi}_{\sigma}(0) = -\bar{\psi}_{\sigma}(\beta) \\ \psi_{\sigma}(0) = -\psi_{\sigma}(\beta)}} D(\bar{\psi}_{\sigma}, \psi_{\sigma}) e^{-S[\bar{\psi}_{\sigma}, \psi_{\sigma}]}$$

$$S[\bar{\psi}_{\sigma}, \psi_{\sigma}] = \int_{0}^{\beta} d\tau \left[\int d^{d}r \, \bar{\psi}_{\sigma}(\mathbf{r}, \tau) \left(\partial_{\tau} + \frac{\hat{\mathbf{p}}^{2}}{2m} - \mu \right) \psi_{\sigma}(\mathbf{r}, \tau) + \frac{1}{2} \int d^{d}r \int d^{d}r' \bar{\psi}_{\sigma}(\mathbf{r}, \tau) \bar{\psi}_{\sigma'}(\mathbf{r}', \tau) \frac{e^{2}}{|\mathbf{r} - \mathbf{r}'|} \psi_{\sigma'}(\mathbf{r}', \tau) \psi_{\sigma}(\mathbf{r}, \tau) \right]$$

Expressed in Fourier basis: $\psi_{\sigma}(\mathbf{r}, \tau) = \frac{1}{\sqrt{L^3 \beta}} \sum_{\mathbf{k}, \omega_n} e^{i(\mathbf{k} \cdot \mathbf{r} - \omega_n \tau)} \psi_{\mathbf{k}, \omega_n, \sigma}$

$$S = \int_0^\beta d\tau \left[\sum_{\mathbf{k}} \bar{\psi}_{\mathbf{k}\sigma}(\tau) \left(\partial_\tau + \epsilon_{\mathbf{k}} - \mu \right) \psi_{\mathbf{k}\sigma}(\tau) + \frac{1}{2L^d} \sum_{\mathbf{q} \neq 0} \frac{4\pi e^2}{\mathbf{q}^2} \rho_{\mathbf{q}}(\tau) \rho_{-\mathbf{q}}(\tau) \right]$$

where
$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m}$$
 and $\rho_{\mathbf{q}}(\tau) = \int d^d r \, e^{-i\mathbf{q}\cdot\mathbf{r}} \rho(\mathbf{r},\tau) \equiv \sum_{\mathbf{k}} \bar{\psi}_{\mathbf{k}\sigma}(\tau) \psi_{\mathbf{k}+\mathbf{q},\sigma}(\tau)$ (N.B. neutralising background \rightsquigarrow exclusion of $\mathbf{q} = 0$ from sum)

With the action quartic in fermionic fields ψ , \mathcal{Z} can not be evaluated exactly

For weak interaction, $r_s \ll 1$, we could expand in Coulomb interaction: \sim Feynman diagram expansion (cf. Gell-Mann—Brückner theory)

Lecture Notes October 2005

Lecture XVII 50

Alternative — use field integral to isolate leading diagrammatic series expansion — known as the Random Phase Approximation (RPA)

▷ GENERAL PRINCIPLE:

When confronted with interacting field theory, seek decomposition of interaction through introduction of auxiliary field which captures low-energy content of theory

In some cases, these fields are identified with the elementary particles that mediate the interaction (see below); in others, these fields encode the low-energy collective modes of the system (e.g. superfluid, superconductor)

▶ Decoupling facilitated using the <u>Hubbard-Stratonovich transformation</u>:

$$e^{-\int_0^\beta d\tau \sum_{\mathbf{q}\neq 0} \frac{2\pi e^2}{L^d \mathbf{q}^2} \rho_{\mathbf{q}}(\tau) \rho_{-\mathbf{q}}(\tau)} = \int D\phi \ e^{-\int_0^\beta d\tau \sum_{\mathbf{q}\neq 0} \left[\frac{\mathbf{q}^2}{8\pi} \phi_{\mathbf{q}}(\tau) \phi_{-\mathbf{q}}(\tau) + \frac{ie}{2L^{d/2}} (\phi_{\mathbf{q}}(\tau) \rho_{-\mathbf{q}}(\tau) + \rho_{\mathbf{q}}(\tau) \phi_{-\mathbf{q}}(\tau)) \right]}$$

 \triangleright Physically, ϕ represents (scalar) photon field which mediates Coulomb interaction N.B. ϕ real and periodic $\phi(\tau + \beta) = \phi(\tau)$

$$\mathcal{Z} = \int D(\bar{\psi}_{\sigma}, \psi_{\sigma}) \int D\phi \exp \left\{ -\int_{0}^{\beta} d\tau \int d^{d}r \left[\frac{1}{8\pi} \left(\partial \phi \right)^{2} + \bar{\psi}_{\sigma} \left(\partial_{\tau} + \frac{\hat{\mathbf{p}}^{2}}{2m} - \mu + ie\phi \right) \psi_{\sigma} \right] \right\}$$

Gaussian in Grassmann fields, field integral may be performed:

using identity $\int D[\bar{\psi}, \psi] \exp[-\bar{\psi}M\psi] = \det M = \exp[\ln \det M]$

$$\mathcal{Z} = \int D\phi \exp\left[-\int_0^\beta d\tau \int d^d r \frac{1}{8\pi} \left(\partial\phi\right)^2 + \overbrace{2}^{\text{spin}} \ln \det\left(\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu + ie\phi\right)\right]$$

Setting e = 0, photon field decouples from determinant;

recovers partition function of non-interacting electron gas

\triangleright Perturbation Theory in e:

Define free particle Green function: $\hat{G}_0 = [\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu]^{-1}$ and expand: $\ln(1+x) = -\sum_{n=1}^{\infty} (-x)^n/n$

$$\ln \det \left(\partial_{\tau} + \frac{\hat{\mathbf{p}}^{2}}{2m} - \mu + ie\phi \right) \equiv \operatorname{tr} \ln \left(\hat{G}_{0}^{-1} + ie\phi \right) = \operatorname{tr} \ln \hat{G}_{0}^{-1} + \operatorname{tr} \ln \left[1 + ie\hat{G}_{0}\phi \right]$$
$$= \operatorname{tr} \ln \hat{G}_{0}^{-1} - \operatorname{tr} \left[-ie\hat{G}_{0}\phi + \frac{1}{2} \left(ie\hat{G}_{0}\phi \right)^{2} + \cdots \right]$$

• First order term: for convenience, set $k \equiv (\mathbf{k}, \omega_n)$, etc.

$$2\operatorname{tr}[\hat{G}_{0}\phi] = 2\sum_{k} \overbrace{\langle k|\hat{G}_{0}|k\rangle}^{2} \overbrace{\langle k|\phi|k\rangle}^{2} = \frac{2}{\sqrt{L^{3}\beta}} \sum_{k} \frac{1}{-i\omega_{n} + \epsilon_{k} - \mu} \phi_{0} = 0$$

Lecture Notes October 2005

Lecture XVII 51

 $\phi_0 = 0$ due to neutralising background

• Second order term:

$$2 \times \frac{e^2}{2} \operatorname{tr}[\hat{G}_0 \phi]^2 = e^2 \sum_{k,q} \underbrace{\langle k | \hat{G}_0 | k \rangle \langle k | \phi | k + q \rangle \langle k + q | \hat{G}_0 | k + q \rangle \langle k + q | \phi | k \rangle}_{\text{def}} = \frac{e^2}{2} \sum_{q} \Pi(q) \phi_{-q} \phi_q$$

where "density-density" response function,

$$\Pi(q) = \frac{2}{\beta L^3} \sum_{k} \frac{1}{-i\omega_n + \epsilon_{\mathbf{k}} - \mu} \frac{1}{-i\omega_n - i\omega_m + \epsilon_{\mathbf{k}+\mathbf{q}} - \mu}$$

Combined with bare term, to leading order in e^2 (Random Phase Approximation),

$$\mathcal{Z} = \mathcal{Z}_0 \int D\phi \, e^{-S[\phi]}, \qquad S[\phi] = \frac{1}{2} \sum_q \overbrace{\left(\frac{\mathbf{q}^2}{4\pi} - e^2\Pi(q)\right)}^{D^{-1}(q)} |\phi_q|^2 + O(e^4)$$

 \mathcal{Z}_0 denotes partition function of non-interacting gas

 \triangleright Physically, $D^{-1}(q)$ denotes dynamically <u>screened Coulomb interaction</u>

$$D^{-1}(q) = \epsilon(q) \frac{\mathbf{q}^2}{4\pi}, \qquad \epsilon(q) = 1 - \frac{4\pi e^2}{\mathbf{q}^2} \Pi(q)$$

where $\epsilon(q)$ is the energy and momentum dependent effective <u>dielectric function</u>

Diagrammatic interpretation:

$$D(q) = \frac{4\pi}{\mathbf{q}^2} \frac{1}{1 - \frac{4\pi e^2}{\mathbf{q}^2} \Pi(q)} = \frac{4\pi}{\mathbf{q}^2} \sum_{n=0}^{\infty} \left(e^2 \Pi(q) \frac{4\pi}{\mathbf{q}^2} \right)^n$$

Lecture Notes October 2005